NANOELECTRONIC AND NANOMAGNETIC DEVICES FOR REVOLUTIONARY COMPUTING AND SENSOR APPLICATIONS

Final Report

JPL Task 1020

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A. OBJECTIVES

This research effort has focused on the examination of the effects of electro-magnetic fields and many-body interactions on a spin-based nano-device, with the goal of understanding the fundamental characteristics of the novel device and of evaluating its reliability under external perturbations.

B. PROGRESS AND RESULTS

1. Science Data

We have completed the simulations of spin transport, gyro-magnetic ratios, magneto-optical response, and spin decoherence, which are fundamental characteristics of spin-based nano-devices. The itemized simulation results are shown below:

Spin transport across semiconductor heterostructures: Polarized spin precession and relaxation across semiconductor heterostructures is calculated with a spin-diffusion model, motivated by a recent measurement of the spin dynamics in a ZnSe epilayer grown on GaAs. Experiments have shown that the spin precession and relaxation in the ZnSe epilayer are shifting from ZnSe-like to GaAs-like when an electric field is applied between the epilayer and the substrate. We used a spin-diffusion model with a time-dependent transmission coefficient across the interface to account for the thermalization of the electrons excited in the GaAs. Figure 1 illustrates the electric field dependence on the simulated spin dynamics, which is in excellent agreement with experiment. This simulation provides a clear explanation of the dependence of spin transport across semiconductor heterostructures on the electric field [1].

Gyro-magnetic ratio of quantum dots: Various proposed spintronic devices utilize Zeeman splitting (i.e. the energy spacing between the spin up and down states in the presence of a magnetic field) which is determined by the effective gyro-magnetic ratio of the host material. We calculated the gyro-magnetic ratio using the atomistic tight-binding model, which is the theoretical framework of NEMO-3D. Figure 2 shows that the effective gyro-magnetic ratio of InAs quantum dots ranges from 2.0 to 3.5 for different electron states. These values are very different from that of bulk InAs (–14.9) and are in

excellent agreement with recent experiments. The difference is attributed to the large increase of the band gap in a quantum dot relative to the change of the spin-orbit coupling (which is almost identical to the bulk value). This work demonstrates that the gyro-magnetic ratio can be tuned by adjusting the quantum-dot size [2].

Magneto-optical response of quantum dots: The use of quantum dots in optical devices such as lasers and detectors is expected to lead to improved detection properties like low-threshold current density and reduced temperature sensitivity due to the delta-function-like density of states of the dots. It is of particular interest to NASA missions to determine how well the improved optical properties will be preserved and the proposed optical devices will function under extreme conditions. Motivated by this need, we investigated how a high magnetic field affects the optical properties of quantum dots. The transition rate between an electron and hole level exhibits a strong selection rule for electron-hole pair creation and recombination. Only the electron-hole pairs with zero angular momentum difference between their envelope functions yield significant transition rates. Our calculations have shown that this selection rule remains intact even at high magnetic fields (see Fig. 3). The robustness of the selection rule is attributed to the negligible magnetic coupling between states with different angular momenta. To observe a breakdown of the selection rule, we estimate that the magnetic field needs to be as strong as 100 T. This result shows that optical nano-devices are tolerant to high magnetic fields [2].

Spin decoherence in quantum dots: Spin decoherence is one of the key limitations in building a solid-state quantum computer. While several processes are known to contribute to the finite lifetime of spin states, the hyperfine interaction with nuclear spins is identified as a dominant mechanism in III/V semiconductor quantum dots. In the spirit of developing a simulation tool that can model realistic qubits, we modeled the hyperfine induced decoherence using accurate wave functions obtained from NEMO-3D. Recognizing that the interaction process is non-Markovian in the sense that the nuclear system "remembers" prior interaction with the electron spin, we have elected two complementary approaches. First, we have calculated the time-dependent spin correlation function up to first-order perturbation. Figure 4 shows that the average spin polarization in InAs quantum dots decreases with a decoherence time on the order of 1 μs. Although this approach provides a good estimation of the decoherence, it suffers from the limitations that the second-order-perturbation term diverges as time increases, and that arbitrary magnetic fields cannot be included. Our second approach aims at overcoming these shortcomings and relies on a simplified version of the non-equilibrium quantum-field kinetics formalism. This approach has the advantage that the effect of arbitrary time-dependent magnetic fields can be described, enabling the simulation of real quantum-computing operations including decoherence effects. The second approach provides decoherence times close to those obtained with the perturbation approach, confirming the reliability of the first approach for the estimation of decoherence times [3]. This simulation result supports the proposed idea that a quantum dot can be used as a building unit of quantum computers, since the quantum information contained in the spin states of a quantum dot can remain coherent during up to 10^4 information operations.

2. Other Results

This scientific investigation has led to the development of a spin dynamics theory within the non-equilibrium Green function formalism, the development of an efficient boundary condition for the electronic structure of embedded nanostructures, a considerable extension of the simulation scope of NEMO-3D, and the first public release of the NEMO-3D. The itemized results are shown below:

Spin dynamics theory: We have established the fundamental property that for a system of spin-carrying electrons in a magnetic field, the Surface Green Function (SGF), which describes the coupling between the device region and the leads, can be expressed in terms of the SGF of a spin-less system multiplied by a time-dependent factor describing the precession. This finding is an essential prerequisite to the practical implementation of a numerical solution of the spin dynamics within the non-equilibrium Green function formalism. This work demonstrates our growing understanding of spin dynamics in heterostructures, which is a key ingredient in building a comprehensive design tool for quantum computers.

Closed boundary condition: Recognizing that the modeling of the electronic structure of nanostructures embedded in a large buffer is computationally challenging, we have developed an efficient boundary condition that can imitate the large buffer with a truncated buffer. The new boundary condition that raises the energies of dangling bonds at the surface leads to the efficient elimination of mid-gap surface states and to the fast numerical convergence of interior-state energies. The numerical efficiency of NEMO-3D has thereby been greatly enhanced.

NEMO-3D upgrade: We have extended the simulation scope of NEMO-3D by including electric and magnetic fields, many-body interactions, and an efficient boundary condition. The electric and magnetic fields are incorporated into NEMO-3D in a gauge-invariant way without introducing any extra adjustable parameters. As a prototype for many-body interactions, Coulomb interaction (charge-charge interaction) and hyperfine Fermi contact interaction (spin-spin interaction) are included in NEMO-3D. Finally, the newly developed boundary condition was incorporated into NEMO-3D [4,5].

NEMO-3D release: We have completed all the paperwork for public release of NEMO-3D software with JPL/Caltech and are currently completing the full code documentation. The first public alpha version has been released on Oct. 7, 2003 through Open Channel Foundation http://www.openchannelsoftware.com/projects/NEMO_3D.

C. SIGNIFICANCE OF RESULTS

In summary, we have demonstrated with atomistic-level simulation that spin-based devices are tolerant to heterostructure interfaces and high magnetic fields. Our simulation results show that (i) the efficiency of spin injection across semiconductor heterostructures can be tuned by electric fields, (ii) the gyro-magnetic ratio of quantum dots can be tuned by dot sizes, (iii) the optical properties (absorption and recombination rates) of quantum dots are robust even at high magnetic fields, and (iv) quantum dots are ideal candidates for building units of quantum computers due to their long decoherence time on the order of 1 μs.

These studies directly tie into some of NASA's core objectives, such as developing electronic components that are reliable in extreme environments and developing computational capabilities that allow for rapid on-board decision processes, needed, for example, in the EDL (entry, descent, and landing) phase of a planetary exploration mission. Point (iii) is a prime example of how a careful study supports the development of cutting-edge optical detectors using quantum dots (detection range expected from the near-UV to the far-infrared). It demonstrates the robustness of the detection mechanism at magnetic-field strengths endemic, e.g., in the vicinity of Jupiter, where the magnetic field ranges from 0.0005 to 1 T. Missions such as JIMO (Jupiter Icy Moons Orbiter) are expected to significantly benefit from such advances. Points (i), (ii), and (iv) are in full support of the ambitious goal of developing a quantum computer with computational capabilities far beyond current technology. This work is a significant step toward developing the first realistic simulation tool for quantum computers.

Finally, this scientific investigation led to a considerable extension of the simulation scope of NEMO-3D and the first public release of NEMO-3D. We consider the NEMO-3D release as a key contribution to the field of nanoelectronics and a first step towards the realistic simulation of spintronics. This simulator will enable researchers to explore the design space for nanoelectronic and spintronic applications.

D. FINANCIAL STATUS

The total funding for this task was $100,000, all of which has been expended.

E. PERSONNEL

In addition to the personnel listed at the top of this report, K. Birgitta Whaley of University of California at Berkeley and Nick Rizzo, Brad Engel, and Herb Goronkin at Motorola Labs, Physical Sciences Research Laboratory contributed to this task.

F. PUBLICATIONS

[1] Paul von Allmen, Gerhard Klimeck, Fabiano Oyafuso, Nick Rizzo, Brad Engel, and Herb Goronkin, "Interplay of spin precession and spin diffusion across a semiconductor interface", submitted to *Appl. Phys. Lett.* 2003.

[2] Seungwon Lee, Fabiano Oyafuso, Paul von Allmen, Gerhard Klimeck, and K. Birgitta Whaley, "Magneto-optical response of InAs lens-shaped self-assembled quantum dots", accepted for publication in *J. of Computational Electronics,* 2003.

[3] Seungwon Lee, Paul von Allmen, Fabiano Oyafuso, Gerhard Klimeck, and K. Birgitta Whaley, "Electron spin dephasing and decoherence by interaction with nuclear spins in self-assembled quantum dots", accepted in proceedings of *Winter International Symposium on Information and Communication Technologies*, Cancun, Mexico, 5-8 January 2004.

[4] Seungwon Lee, Fabiano Oyafuso, Paul von Allmen, and Gerhard Klimeck, "Boundary conditions for the electronic structure of finite-extent, embedded semiconductor nanostructures with empirical tight-binding model", submitted to Phys. Rev. B. 2003.

[5] Seungwon Lee, Fabiano Oyafuso, Paul von Allmen, and Gerhard Klimeck, "Numerical surface treatment for finite-extent semiconductor nanostructures", in proceedings of *14th Workshop on Modeling and Simulation of Electron Devices*, Barcelona, Spain, 16-17 October 2003.

G. FIGURES

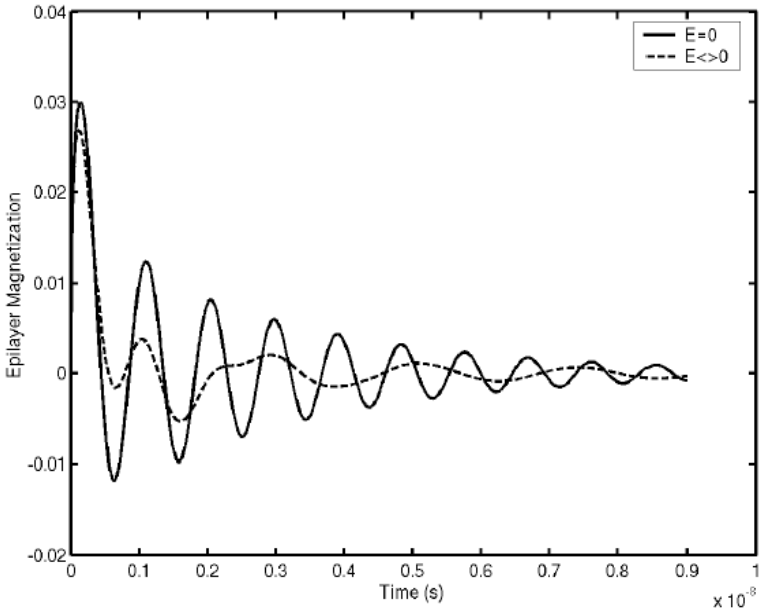

Figure 1. Time evolution of the spin magnetization in a ZnSe epilayer grown on a GaAs substrate both with and without an electric field E. Without the electric field, the spin evolution is determined solely by ZnSe parameters. With the electric field, the spin dynamics evolves from ZnSe-like to GaAs-like [1].

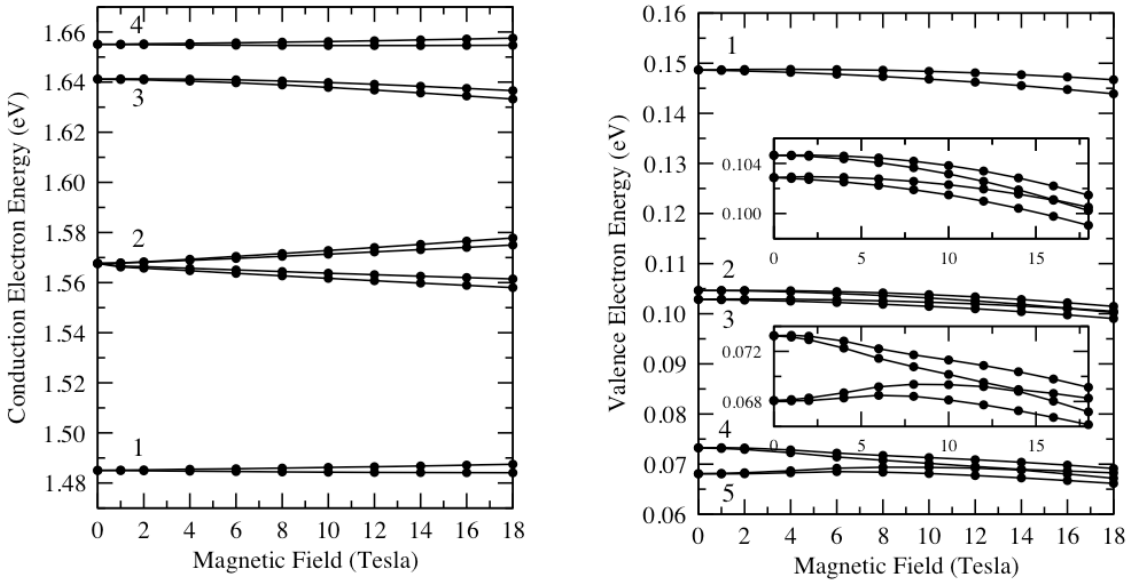

Figure 2. Conduction and valence electron energies versus magnetic field along the growth direction of InAs self-assembled quantum dots with diameter 10 nm and height 2 nm. For conduction electron states, the Zeeman splitting between the spin up and down states scales linearly with magnetic field, yielding an effective gyro-magneto ratio ranging from 2.0 to 3.5. For valence electron states, the Zeeman splitting demonstrates a nonlinear response to the magnetic field [2].

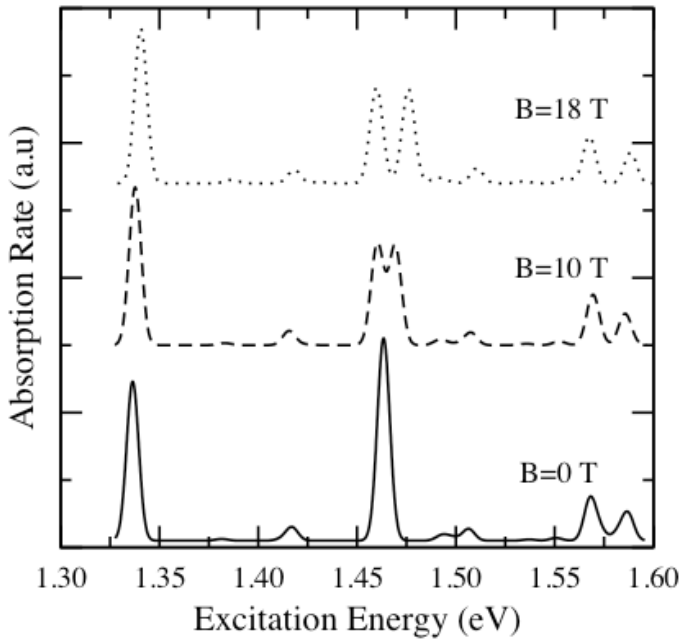

Figure 3. Absorption rate versus excitation energy for InAs self-assembled quantum dots with diameter 10 nm and height 2 nm with various magnetic fields B. Only the electron-hole pairs with zero angular momentum difference exhibit strong absorption rates. Magnetic fields split the absorption peaks due to the Zeeman splitting, but preserve the selection rule of the absorption rates [2].

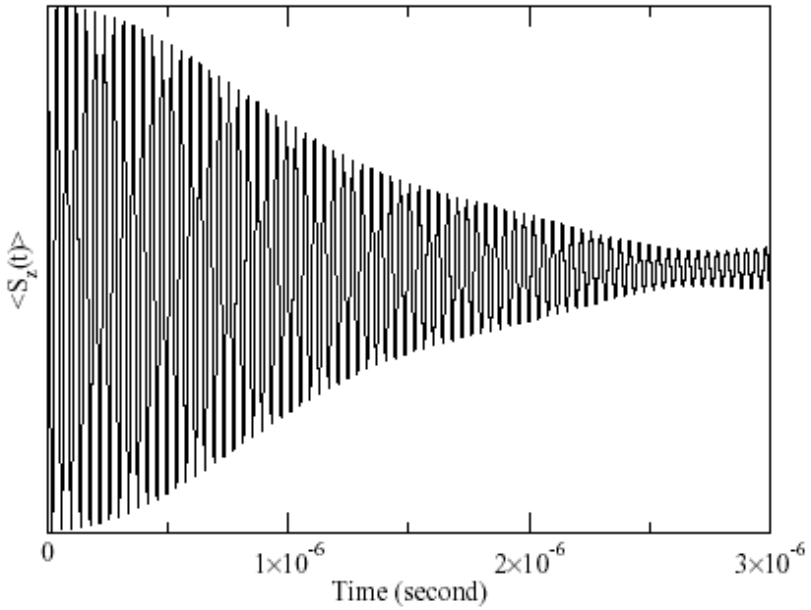

Figure 4. Time evolution of average electron-spin polarization under the hyperfine interaction with about 30000 nuclear spins in an InAs self-assembled quantum dot. The average spin polarization decreases exponentially with a decoherence time on the order of 1 μs [3].